International Tables for Crystallography (2013). Vol. D, Section 1.2.7.2, pp. 64–66.

Table 1.2.6.10 (*cont.*)

(h) $D_2 \times C_2$

$A^2 = -E, B^2 = C^2 = (AB)^2 = E, AC = CA, BC = CB$								
Elements	E	A	B	AB	C	AC	BC	ABC
Γ'_9	2	0	0	0	2	0	0	0
Γ'_{10}	2	0	0	0	−2	0	0	0
$A^2 = E, B^2 = C^2 = (AB)^2 = E, AC = -CA, BC = CB$								
Elements	E	A	B	AB	C	AC	BC	ABC
Γ'_{11}	2	0	2	0	0	0	0	0
Γ'_{12}	2	0	−2	0	0	0	0	0
$A^2 = E, B^2 = C^2 = (AB)^2 = E, AC = CA, BC = -CB$								
Elements	E	A	B	AB	C	AC	BC	ABC
Γ'_{13}	2	$2i$	0	0	0	0	0	0
Γ'_{14}	2	$-2i$	0	0	0	0	0	0
$A^2 = -E, B^2 = C^2 = (AB)^2 = E, AC = -CA, BC = CB$								
Elements	E	A	B	AB	C	AC	BC	ABC
Γ'_{15}	2	0	0	0	0	0	2	0
Γ'_{16}	2	0	0	0	0	0	−2	0
$A^2 = -E, B^2 = C^2 = (AB)^2 = E, AC = CA, BC = -CB$								
Elements	E	A	B	AB	C	AC	BC	ABC
Γ'_{17}	2	0	0	0	0	$2i$	0	0
Γ'_{18}	2	0	0	0	0	$-2i$	0	0
$A^2 = E, B^2 = C^2 = (AB)^2 = E, AC = -CA, BC = -CB$								
Elements	E	A	B	AB	C	AC	BC	ABC
Γ'_{19}	2	0	0	$2i$	0	0	0	0
Γ'_{20}	2	0	0	$-2i$	0	0	0	0
$A^2 = -E, B^2 = C^2 = (AB)^2 = E, AC = -CA, BC = -CB$								
Elements	E	A	B	AB	C	AC	BC	ABC
Γ'_{21}	2	0	0	0	0	0	0	$2i$
Γ'_{22}	2	0	0	0	0	0	0	$-2i$

cyclotomics. Use of arbitrary real numbers would imply a finite precision.

Detailed instructions for the use of the program, together with a guided tour (*QuickStart*), can be found in the manual for the program.

1.2.7.2. *Tensors*

The tensor module of *Tenχar* determines the number of independent elements and the relations between the elements of tensors and pseudotensors invariant under a chosen point group and with specified permutation symmetry of the indices. Although the list of point groups provided in a database is limited to dimensions two and three, the program runs for arbitrary dimensions. Similarly, the choice of index permutation symmetry is limited to rank smaller than or equal to four. This is also not a restriction of the program, which works for arbitrary rank. For higher dimensions and higher ranks, the user needs to provide additional information. The limiting factors are in fact the speed, which becomes low for higher dimensions and/or higher rank, and the available memory, which must be sufficient to store the tensor elements.

When the program is started and the tensor part is chosen *via* a button, a selection box opens. The user can specify dimension and rank in open fields. A field without a coloured border has a formally correct content, but the user should check whether the pregiven numbers correspond to his wishes. In open fields with a coloured border, additional information must be given. Clicking on the button ‘point group’ results in the opening of a new selection window. A specific two- or three-dimensional point group may be chosen *via* geometric crystal classes. This point group may be viewed if wished. The chosen point group is given by generating matrices and is the one under which the (pseudo)tensor is invariant.

The second symmetry is the index permutation symmetry. For tensors and pseudotensors up to rank four, all possible symmetries are tabulated after clicking ‘permutation symmetry’. The indices are numbered from 0 to $r - 1$, where r is the rank. The symbol for a tensor symmetric in the indices 2 and 3 is (2 3), and it is [2 3] if the tensor gets a minus sign under permutation. Arbitrary combinations of symmetric and antisymmetric series can be made. For example, (0 1) 2 [3 4] is a rank-five tensor which is symmetric in the first two indices and antisymmetric in the last two indices. The symbol (0 1 2) characterizes a rank-three tensor that is fully symmetric in all indices. For (pseudo)tensors of rank five and higher, the user needs to specify the permutation symmetry using parentheses in this way. Symmetrization of other pairs is similar. For example, if the rank-three tensor T is symmetric in the first and last indices, the symbol for its permutation character is (0 2) 1. Then $T_{xyz} = T_{zyx}$.

Different settings of the point group may be specified. The standard setting of a point group as given in *International Tables for Crystallography* Volume A may be different from the one to be specified. In this case, the user may perform a basis transformation which transforms the standard setting to the desired setting. This is done *via* the button ‘basis transformation’. The standard setting is chosen with ‘no transformation’. The transformation from a hexagonal to an orthogonal (Cartesian) basis is performed by selecting ‘hC transformation’.

Finally, the tensor or pseudotensor with the specified point group and permutation symmetry is calculated and displayed in a (numbered) window. The command for this is given by clicking on the button ‘tensor’ or ‘pseudotensor’, respectively. In the window appear the input data, such as the point group, the

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Table 1.2.6.11. *Special points in the Brillouin zones in three dimensions*

(*a*) Triclinic

k		$K_{\mathbf{k}}$	Kovalev
a	000	$\bar{1}$	k_8
b	$00\frac{1}{2}$	$\bar{1}$	k_7
c	$0\frac{1}{2}0$	$\bar{1}$	k_6
d	$\frac{1}{2}00$	$\bar{1}$	k_5
e	$\frac{1}{2}\frac{1}{2}0$	$\bar{1}$	k_4
f	$\frac{1}{2}0\frac{1}{2}$	$\bar{1}$	k_3
g	$0\frac{1}{2}\frac{1}{2}$	$\bar{1}$	k_2
h	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$\bar{1}$	k_1

(*b*) Monoclinic *P*

k		$K_{\mathbf{k}}$	Kovalev
a	000	$2/m$	k_7
b	$00\frac{1}{2}$	$2/m$	k_{11}
c	$\frac{1}{2}00$	$2/m$	k_{12}
d	$0\frac{1}{2}0$	$2/m$	k_{13}
e	$0\frac{1}{2}\frac{1}{2}$	$2/m$	k_9
f	$\frac{1}{2}0\frac{1}{2}$	$2/m$	k_8
g	$\frac{1}{2}\frac{1}{2}0$	$2/m$	k_{14}
h	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$2/m$	k_{10}
i	00γ	2	k_3
j	$0\frac{1}{2}\gamma$	2	k_5
k	$\frac{1}{2}0\gamma$	2	k_4
l	$\frac{1}{2}\frac{1}{2}\gamma$	2	k_6
m	$\alpha\beta0$	m	k_1
n	$\alpha\beta\frac{1}{2}$	m	k_2

(*c*) Monoclinic *A*

k		$K_{\mathbf{k}}$	Kovalev
a	000	$2/m$	k_6
b	010	$2/m$	k_8
c	$\frac{1}{2}00$	$2/m$	k_7
d	$\frac{1}{2}10$	$2/m$	k_9
e	$0\frac{1}{2}\frac{1}{2}$	$\bar{1}$	k_4
f	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$\bar{1}$	k_5
g	00γ	2	k_2
h	$\frac{1}{2}0\gamma$	2	k_3
i	$\alpha\beta0$	m	k_1

(*d*) Orthorhombic *P*

k		$K_{\mathbf{k}}$	Kovalev
a	000	mmm	k_{19}
b	$\frac{1}{2}00$	mmm	k_{20}
c	$00\frac{1}{2}$	mmm	k_{22}
d	$\frac{1}{2}0\frac{1}{2}$	mmm	k_{24}
e	$0\frac{1}{2}0$	mmm	k_{21}
f	$\frac{1}{2}\frac{1}{2}0$	mmm	k_{25}
g	$0\frac{1}{2}\frac{1}{2}$	mmm	k_{23}
h	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	mmm	k_{26}
i	$\alpha00$	$2mm$	k_7
j	$\alpha0\frac{1}{2}$	$2mm$	k_{12}
k	$\alpha\frac{1}{2}0$	$2mm$	k_{10}
l	$\alpha\frac{1}{2}\frac{1}{2}$	$2mm$	k_{11}
m	$0\beta0$	$m2m$	k_8
n	$0\beta\frac{1}{2}$	$m2m$	k_{15}
o	$\frac{1}{2}\beta0$	$m2m$	k_{13}
p	$\frac{1}{2}\beta\frac{1}{2}$	$m2m$	k_{14}
q	00γ	$mm2$	k_9
r	$0\frac{1}{2}\gamma$	$mm2$	k_{18}
s	$\frac{1}{2}0\gamma$	$mm2$	k_{16}
t	$\frac{1}{2}\frac{1}{2}\gamma$	$mm2$	k_{17}
u	$0\beta\gamma$	m	k_1
v	$\frac{1}{2}\beta\gamma$	$m11$	k_2
w	$\alpha0\gamma$	$1m1$	k_3
x	$\alpha\frac{1}{2}\gamma$	$1m1$	k_4
y	$\alpha\beta0$	$11m$	k_5
z	$\alpha\beta\frac{1}{2}$	$11m$	k_6

(*e*) Orthorhombic *C*

k		$K_{\mathbf{k}}$	Kovalev
a	000	mmm	k_{14}
b	010	mmm	k_{15}
c	$01\frac{1}{2}$	mmm	k_{17}
d	$00\frac{1}{2}$	mmm	k_{16}
e	$\frac{1}{2}\frac{1}{2}0$	$2/m$	k_{12}
f	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$2/m$	k_{13}
g	$\alpha00$	$2mm$	k_8
h	$\alpha0\frac{1}{2}$	$2mm$	k_9
i	$0\beta0$	$m2m$	k_{10}
j	$0\beta\frac{1}{2}$	$m2m$	k_{11}
k	00γ	$mm2$	k_6
l	01γ	$mm2$	k_7
m	$\frac{1}{2}\frac{1}{2}\gamma$	112	k_5
n	$0\beta\gamma$	$m11$	k_1
o	$\alpha0\gamma$	$1m1$	k_2
p	$\alpha\beta0$	$11m$	k_3
q	$\alpha\beta\frac{1}{2}$	$11m$	k_4

(*f*) Orthorhombic *I*

k		$K_{\mathbf{k}}$	Kovalev
a	000	mmm	k_{17}
b	001	mmm	k_{18}
c	$0\frac{1}{2}\frac{1}{2}$	$2/m11$	k_{13}
	$1\frac{1}{2}\frac{1}{2}$	$2/m11$	k_{10}
d	$\frac{1}{2}0\frac{1}{2}$	$12/m1$	k_{14}
	$\frac{1}{2}1\frac{1}{2}$	$12/m1$	k_{11}
e	$\frac{1}{2}\frac{1}{2}0$	$112/m$	k_{15}
	$\frac{1}{2}\frac{1}{2}1$	$112/m$	k_{12}
f	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	222	k_{16}
g	$\alpha00$	$2mm$	k_7
h	$0\beta0$	$m2m$	k_8
i	00γ	$mm2$	k_9
j	$\frac{1}{2}\frac{1}{2}\gamma$	112	k_6
k	$\frac{1}{2}\beta\frac{1}{2}$	121	k_5
l	$\alpha\frac{1}{2}\frac{1}{2}$	211	k_4
m	$0\beta\gamma$	$m11$	k_1
n	$\alpha0\gamma$	$1m1$	k_2
o	$\alpha\beta0$	$11m$	k_3

(*g*) Orthorhombic *F*

k		$K_{\mathbf{k}}$	Kovalev
a	000	mmm	k_{14}
b	100	mmm	k_{15}
c	010	mmm	k_{16}
d	001	mmm	k_{17}
e	$\alpha00$	$2mm$	k_4
f	$\alpha10$	$2mm$	k_5
g	$0\beta0$	$m2m$	k_6
h	$1\beta0$	$m2m$	k_7
i	00γ	$mm2$	k_8
j	01γ	$mm2$	k_9
k	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$\bar{1}$	k_{10}
	$-\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$\bar{1}$	k_{11}
	$\frac{1}{2}-\frac{1}{2}\frac{1}{2}$	$\bar{1}$	k_{12}
	$\frac{1}{2}\frac{1}{2}-\frac{1}{2}$	$\bar{1}$	k_{13}
l	$0\beta\gamma$	$m11$	k_1
m	$\alpha0\gamma$	$1m1$	k_2
n	$\alpha\beta0$	$11m$	k_3

(*h*) Tetragonal *P*

k		$K_{\mathbf{k}}$	Kovalev
a	000	$4/mmm$	k_{17}
b	$00\frac{1}{2}$	$4/mmm$	k_{19}
c	$\frac{1}{2}\frac{1}{2}0$	$4/mmm$	k_{18}
d	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$4/mmm$	k_{20}
e	$0\frac{1}{2}\frac{1}{2}$	mmm	k_{16}
f	$0\frac{1}{2}0$	mmm	k_{15}
g	00γ	$4mm$	k_{13}
h	$\frac{1}{2}\frac{1}{2}\gamma$	$4mm$	k_{14}
i	$0\frac{1}{2}\gamma$	$mm2$	k_{12}
j	$\alpha\alpha0$	$2mm$	k_{10}
k	$\alpha\alpha\frac{1}{2}$	$2mm$	k_{11}
l	$0\beta0$	$m2m$	k_8
m	$0\beta\frac{1}{2}$	$m2m$	k_9
n	$\alpha\frac{1}{2}0$	$2mm$	k_6
o	$\alpha\frac{1}{2}\frac{1}{2}$	$2mm$	k_7
p	$\alpha\beta0$	$11m$	k_1
q	$\alpha\beta\frac{1}{2}$	$11m$	k_2
r	$\alpha\alpha\gamma$	m	k_5
s	$0\beta\gamma$	$m11$	k_3
t	$\alpha\frac{1}{2}\gamma$	$1m1$	k_4

(*i*) Tetragonal *I*

k		$K_{\mathbf{k}}$	Kovalev
a	000	$4/mmm$	k_{14}
b	001	$4/mmm$	k_{15}
c	$\frac{1}{2}\frac{1}{2}0$	mmm	k_{13}
d	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$\bar{4}m2$	k_{12}
e	00γ	$4mm$	k_{10}
f	$\frac{1}{2}0\frac{1}{2}$	$12/m1$	k_{11}
g	$\frac{1}{2}\frac{1}{2}\gamma$	$2mm$	k_9
h	$\alpha\alpha0$	$2mm$	k_7
i	$\alpha00$	$2mm$	k_7
j	$\alpha(1-\alpha)0$	$2mm$	k_8
k	$\frac{1}{2}\beta\frac{1}{2}$	121	k_5
l	$\alpha\beta0$	$11m$	k_2
m	$\alpha\alpha\gamma$	m	k_3
	$\alpha(1-\alpha)\gamma$	m	k_4
n	$\alpha0\gamma$	$1m1$	k_1

(*j*) Trigonal *R* (rhombohedral axes)

k		$K_{\mathbf{k}}$	Kovalev
a	000	$\bar{3}m$	k_7
b	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$\bar{3}m$	k_8
c	$\alpha\alpha\alpha$	$3m$	k_6
d	$00\frac{1}{2}$	$2/m$	k_4
e	$\frac{1}{2}\frac{1}{2}0$	$2/m$	k_5
f	$\alpha(-\alpha)0$	2	k_2
g	$\alpha(-\alpha)\frac{1}{2}$	2	k_2
h	$\alpha\beta\beta$	m	k_1

Table 1.2.6.11 (*cont.*)

(*k*) Hexagonal *P*

k		$K_{\mathbf{k}}$	Kovalev
a	000	$6/mmm$	k_{16}
b	$00\frac{1}{2}$	$6/mmm$	k_{17}
c	$\frac{1}{3}\frac{1}{3}0$	$\bar{6}m2$	k_{13}
d	$\frac{1}{3}\frac{1}{3}\frac{1}{2}$	$\bar{6}m2$	k_{15}
e	00γ	$6mm$	k_{11}
f	$\frac{1}{2}00$	mmm	k_{12}
g	$\frac{1}{2}0\frac{1}{2}$	mmm	k_{14}
h	$\frac{1}{3}\frac{1}{3}\gamma$	$3m$	k_{10}
i	$\frac{1}{2}0\gamma$	$2mm$	k_9
j	$\alpha 00$	$2mm$	k_5
k	$\alpha 0\frac{1}{2}$	$2mm$	k_7
l	$\alpha\alpha 0$	$2mm$	k_6
m	$\alpha\alpha\frac{1}{2}$	$2mm$	k_8
n	$\alpha 0\gamma$	m	k_3
o	$\alpha\alpha\gamma$	m	k_4
p	$\alpha\beta 0$	m	k_1
q	$\alpha\beta\frac{1}{2}$	m	k_2

(*l*) Cubic *P*

k		$K_{\mathbf{k}}$	Kovalev
a	000	$m\bar{3}m$	k_{12}
b	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$m\bar{3}m$	k_{13}
c	$\frac{1}{2}\frac{1}{2}0$	$4/mmm$	k_{11}
d	$00\frac{1}{2}$	$4/mmm$	k_{10}
e	00γ	$4mm$	k_8
f	$\frac{1}{2}\frac{1}{2}\gamma$	$4mm$	k_7
g	$\alpha\alpha\alpha$	$3m$	k_9
h	$\frac{1}{2}0\gamma$	$mm2$	k_6
i	$\alpha\alpha 0$	$2mm$	k_4
j	$\alpha\alpha\frac{1}{2}$	$2mm$	k_5
k	$\alpha\beta 0$	$11m$	k_1
l	$\alpha\beta\frac{1}{2}$	$11m$	k_2
m	$\alpha\alpha\gamma$	m	k_3

(*m*) Cubic *F*

k		$K_{\mathbf{k}}$	Kovalev
a	000	$m\bar{3}m$	k_{11}
b	001	$4/mmm$	k_{10}
c	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$\bar{3}m$	k_9
d	$10\frac{1}{2}$	$\bar{4}m2$	k_8
e	$\alpha 00$	$4mm$	k_6
f	$\alpha\alpha\alpha$	$3m$	k_5
g	$\alpha 01$	$2mm$	k_7
h	$\alpha\alpha 0$	$2mm$	k_4
i	$\alpha(1-\alpha)\frac{1}{2}$	2	k_3
j	$\alpha\beta$	$11m$	k_1
k	$\alpha\alpha\gamma$	m	k_2

(*n*) Cubic *I*

k		$K_{\mathbf{k}}$	Kovalev
a	000	$m\bar{3}m$	k_{11}
b	001	$m\bar{3}m$	k_{10}
c	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$\bar{4}3m$	k_{10}
d	$\frac{1}{2}\frac{1}{2}0$	mmm	k_9
e	$\alpha 00$	$4mm$	k_8
f	$\alpha\alpha\alpha$	$3m$	k_7
g	$\alpha\frac{1}{2}\frac{1}{2}$	$2mm$	k_6
h	$\alpha\alpha 0$	$2mm$	k_4
i	$\alpha(1-\alpha)0$	$2mm$	k_9
j	$\alpha\beta$	$11m$	k_1
k	$\alpha\alpha\gamma$	m	k_2
	$\alpha(1-\alpha)\gamma$	m	k_3

Table 1.2.6.12. *Magnetic point groups*

Type I	Type II	Type III
1	$1'$	
$\bar{1}$	$\bar{1}1'$	$\bar{1}'$
2	$21'$	$2'$
m	$m1'$	m'
$2/m$	$21'/m$	$2'/m,\ 2/m',\ 2'/m',$
222	$2221'$	$2'2'$
$2mm$	$2mm1'$	$2'mm',\ 2m'm'$
mmm	$mmm1'$	$m'mm,\ m'm'm,\ m'm'm'$
4	$41'$	$4'$
$\bar{4}$	$\bar{4}1'$	$\bar{4}'$
$4/m$	$41'/m$	$4'/m,\ 4/m',\ 4'/m'$
422	$4221'$	$4'22',\ 42'2'$
$4mm$	$4mm1'$	$4'mm',\ 4m'm'$
$\bar{4}2m$	$\bar{4}2m1'$	$\bar{4}'2'm,\ \bar{4}'2m',\ \bar{4}2'm'$
$4/mmm$	$4/mmm1'$	$4/m'mm,\ 4'/mm'm,\ 4'/m'm'm,\ 4/mm'm',\ 4/m'm'm'$
3	$31'$	
$\bar{3}$	$\bar{3}1'$	$\bar{3}'$
32	$321'$	$32'$
$3m$	$3m1'$	$3m'$
$\bar{3}m$	$\bar{3}m1'$	$\bar{3}'m,\ \bar{3}'m',\ \bar{3}m'$
6	$61'$	$6'$
$\bar{6}$	$\bar{6}1'$	$\bar{6}'$
$6/m$	$61'/m$	$6'/m,\ 6/m',\ 6'/m'$
622	$6221'$	$6'22',\ 62'2'$
$6mm$	$6mm1'$	$6'mm',\ 6m'm'$
$\bar{6}2m$	$\bar{6}2m1'$	$\bar{6}'2'm,\ \bar{6}'2m',\ \bar{6}2'm'$
$6/mmm$	$6/mmm1'$	$6/m'mm,\ 6'/mm'm,\ 6'/m'm'm,\ 6/mm'm',\ 6/m'm'm'$
23	$231'$	
$m\bar{3}$	$m\bar{3}1'$	$m'\bar{3}$
432	$4321'$	$4'32'$
$\bar{4}3m$	$\bar{4}3m1'$	$\bar{4}'3m'$
$m\bar{3}m$	$m\bar{3}m1'$	$m'\bar{3}m,\ m\bar{3}m',\ m'\bar{3}m'$

dimension, the rank, the permutation symmetry and the setting basis transformation, and the calculated data: the number of independent elements (f) and the relations of these elements. They are either zero or expressed in terms of the free parameters $a_0, \ldots, a_{f-1}$. The tensor elements are given by sequences $x, y, z, \ldots$. The four elements of a general rank-two tensor in two dimensions are xx, xy, yx, yy, corresponding to T_{11}, T_{12}, T_{21} and T_{22}, respectively.

1.2.7.3. *Characters*

Calculations with characters of representations of point groups can be done in the character module of the program. It is selected in the main window by clicking 'character'. A selection window opens in which a point group may be selected just as in the tensor module. The point groups are organized according to dimension and geometric crystal class. Selection of a point group leads to the display of the character table if one asks for it by selecting 'view character table'.

The character table consists of a square array of (complex) numbers. The number of rows is the number of nonequivalent irreducible representations and is equal to the number of columns, which is the number of conjugacy classes of the group. For crystallographic groups, the complex numbers that form the entries of the character table are cyclotomic numbers. These are linear combinations with fractions as coefficients of complex numbers of the form $\exp(2\pi in/m)$. For example, the square root of -1 (i) can be written as $\exp(2\pi i1/4)$. A real number like $\sqrt{2}$ can be written as

$$\sqrt{2} = \tfrac{1}{2}\sqrt{2}(1 + i + 1 - i) = \exp(2\pi i\tfrac{1}{8}) + \exp(2\pi i\tfrac{7}{8}).$$

Another example is

$$\sqrt{5} = 1 + 2\exp(2\pi i\tfrac{1}{5}) + 2\exp(2\pi i\tfrac{4}{5}).$$